

New Type of Hamiltonians Without Ultraviolet Divergence for Quantum Field Theories

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Abstract

We propose a novel type of Hamiltonians for quantum field theories. They are mathematically well-defined (and in particular, ultraviolet finite) without any ultraviolet cut-off such as smearing out the particles over a nonzero radius; rather, the particles are assigned radius zero. We describe explicit examples of such Hamiltonians. Their definition, which is best expressed in the particle–position representation of the wave function, involves a novel type of boundary condition on the wave function, which we call an *interior–boundary condition*. The relevant configuration space is one of a variable number of particles, and the relevant boundary consists of the configurations with two or more particles at the same location. The interior–boundary condition relates the value (or derivative) of the wave function at a boundary point to the value of the wave function at an interior point (here, in a sector of configuration space corresponding to a lesser number of particles).

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1 Introduction

In most quantum field theories (QFTs), the formulas that one obtains for the Hamiltonian (by means of quantization or other heuristics) contain terms for the creation and annihilation of particles that are mathematically ill-defined; for example, they can be written as integrals over all wave vectors $\mathbf{k} \in \mathbb{R}^3$, but the integral is divergent at $|\mathbf{k}| \rightarrow \infty$ (“ultraviolet (UV) divergent”). The problem can be avoided by discretizing space or treating the electron (and other particles) not as a point but smearing it out instead over a small positive radius (“UV regularization” or “UV cut-off”); however, these procedures tend to break the Lorentz invariance, and there is no empirical evidence for either discrete space or a positive electron radius.

We describe a novel way of defining a Hamiltonian for a QFT and report that we have proven for some model QFTs, in joint work with Jonas Lampart and Julian Schmidt [9, 10, 11], that such Hamiltonians are well-defined and self-adjoint. In our approach, space is continuous (as opposed to a lattice), and the radius of the electron (or other particles) is zero. The key element of the approach is a new type of boundary condition that has not been considered before in either physics or mathematics, as far as we

know; it was first considered by one of us in [18] for a different purpose. We call this condition an *interior-boundary condition (IBC)* because it relates the values of ψ on the boundary of configuration space \mathcal{Q} to the values in the interior of \mathcal{Q} , as we will explain presently. The IBC is formulated in the *particle-position representation* of the state vector ψ in Hilbert space \mathcal{H} . Here, “particle representation” means that \mathcal{H} is represented as a Fock space (or, if appropriate, a tensor product of several Fock spaces), and “position representation” that the contribution from the n -particle sector of Fock space is represented (like a wave function in quantum mechanics) as a function of n points in 3-dimensional physical space. Specifically, if \mathcal{H} is a single Fock space then the $\psi \in \mathcal{H}$ can be viewed as a function on a configuration space of a variable number of particles, such as

$$\mathcal{Q} = \bigcup_{n=0}^{\infty} \mathcal{Q}_n = \bigcup_{n=0}^{\infty} [(\mathbb{R}^3)^n \setminus \Delta_n], \quad (1)$$

see Figure 1, where

$$\Delta_n = \left\{ (\mathbf{x}_1, \dots, \mathbf{x}_n) \in (\mathbb{R}^3)^n : \mathbf{x}_i = \mathbf{x}_j \text{ for some } i \neq j \right\} \quad (2)$$

is the “diagonal,” i.e., the set of collision configurations (i.e., those with two or more particles in the same location). The relevant boundary $\partial\mathcal{Q}$ of \mathcal{Q} is $\cup_{n=0}^{\infty} \Delta_n$; the IBC relates the values of ψ on $\partial\mathcal{Q}_n = \Delta_n$ to the values of ψ in the interior of \mathcal{Q}_{n-1} , namely at the configuration with one particle removed (or possibly with more than one particle removed, if more than two particles collide).

Our approach, which we call the IBC approach, provides a Hamiltonian H_{IBC} whose domain is defined using an IBC. It is often assumed that the Hamiltonian of a QFT is the sum of two self-adjoint operators, the free Hamiltonian and the interaction Hamiltonian. In contrast, it is a feature of the IBC approach that its Hamiltonian H_{IBC} cannot be split in this way, as we will explain in detail below.

Work in progress on Hamiltonians with interior-boundary conditions includes [9, 16, 10, 11, 5, 7, 17]. Mathematical proofs are provided in [9, 10, 11]; we give a gentle introduction to IBCs and the ideas behind them in [16].

We hope to apply the IBC approach to quantum electrodynamics and other serious theories in the future; work on implementing IBCs for the Dirac equation is in progress [11]. For the time being, we report results for simple non-relativistic model QFTs. We describe examples of IBCs and how they help define a Hamiltonian, results about the rigorous existence and self-adjointness of the Hamiltonians, and how these Hamiltonians are related to some known cases in which a UV cut-off can be removed, thus making it plausible that the IBC Hamiltonians are physically relevant and not merely mathematical curiosities. Specifically, we consider two models: In Model 1, x -particles can emit and absorb y -particles, and both kinds of particles are non-relativistic; we give the full definition in Section 2 below. Model 2 is a simplified version of Model 1 in which the x -particles cannot move but are fixed at certain locations; this arises as a limiting case of Model 1 in which the mass m_x of the x -particle tends to ∞ ; for simplicity, we

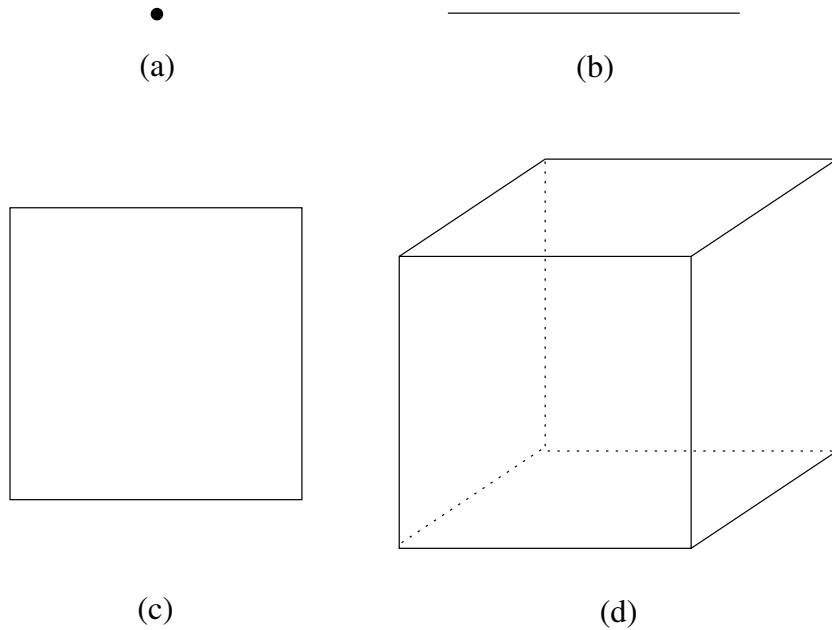


Figure 1: Illustration of a configuration space for a variable number of particles in 1 dimension: (a) The 0-particle sector contains only one configuration, the empty configuration; (b) the 1-particle sector is a copy of physical space; (c) the 2-particle sector; (d) the 3-particle sector. In this example, we have not removed the diagonal Δ_n .

consider only a single x -particle (and call its location the origin). That is, y -particles can be created and annihilated at the origin of \mathbb{R}^3 . For Model 2 (the one with fixed x -particles), it is known that, after a UV cut-off is introduced, the cut-off can be removed by means of a suitable limiting procedure (renormalization), and we can show that the limiting Hamiltonian H_∞ thus obtained coincides with H_{IBC} up to addition of a finite constant (see Section 3.6 below). For Model 1, however, such a procedure is not known (although it is for a similar model [14]). We are currently investigating whether the IBC approach provides, also for Model 1, a well-defined and self-adjoint Hamiltonian without a renormalization procedure [10].

This paper is organized as follows. In Section 2, we describe two simple models of non-relativistic QFT. In Section 3, we describe for each of the two models how to set up an IBC and the corresponding Hamiltonian. In Section 4, we develop a general theory of IBCs under the simplifying assumption that the boundary has codimension 1; this assumption is actually not satisfied in the application to QFT without UV divergence, but Section 4 adds to the full picture about IBCs.

2 Two Models of Non-Relativistic QFT

In this section, we describe two simple non-relativistic model QFTs. We set up their Hilbert spaces \mathcal{H} , describe their original Hamiltonians H_{orig} , and explain why they are UV divergent. Model 1 is a natural, physically reasonable model, while Model 2 is an artificially simplified version that will be useful for an easy discussion of IBCs. In Section 3, we will describe, for each of the two models, our alternative definition of the Hamiltonian involving an interior-boundary condition.

2.1 Model 1: x -Particles Emit and Absorb y -Particles

Model 1 is a QFT adapted from [15, p. 339], [14], and the Lee model [12]. It involves two species of particles, x and y ; the x -particles can emit and absorb y -particles. For simplicity, we take both species to be spinless and assume the non-relativistic dispersion relation $E = \mathbf{p}^2/2m$ for both the x and the y -particles with masses $m_x, m_y > 0$. The Hilbert space is a tensor product of Fock spaces,

$$\mathcal{H} = \mathcal{F}^- \otimes \mathcal{F}^+ \quad (3)$$

with

$$\mathcal{F}^\pm = \bigoplus_{n=0}^{\infty} S_\pm L^2(\mathbb{R}^3, \mathbb{C})^{\otimes n}, \quad (4)$$

where S_- is the anti-symmetrization operator, S_+ is the symmetrization operator, and $S_\pm L^2(\cdots)$ are their ranges (i.e., the spaces of (anti-)symmetric functions on $(\mathbb{R}^3)^n$). Here, we take x -particles to be fermions and y -particles to be bosons.¹ \mathbb{R}^3 is understood as physical space, i.e., ordinary position space. In the following, we simply write $L^2(\mathbb{R}^3)$ for $L^2(\mathbb{R}^3, \mathbb{C})$. A vector $\Psi \in \mathcal{H}$ can be regarded as a function

$$\psi : \mathcal{Q}_x \times \mathcal{Q}_y \rightarrow \mathbb{C} \quad (5)$$

with $\mathcal{Q}_x = \mathcal{Q}_y$ the configuration space of a variable number of particles,

$$\mathcal{Q}_x = \mathcal{Q}_y = \bigcup_{n=0}^{\infty} \mathcal{Q}_n = \bigcup_{n=0}^{\infty} (\mathbb{R}^3)^n, \quad (6)$$

where the union is understood as a disjoint union and $(\mathbb{R}^3)^0 = \{\emptyset\}$. We will discuss removing the collision configurations later.

We call the function ψ the *particle-position representation* of the vector $\Psi \in \mathcal{H}$. A generic element of $\mathcal{Q}_x \times \mathcal{Q}_y$ can be written as $(x, y) = (\mathbf{x}_1, \dots, \mathbf{x}_m, \mathbf{y}_1, \dots, \mathbf{y}_n)$, where bold-face symbols denote vectors in 3-space, while x denotes a configuration of x -particles and y one of y -particles; we will often write x^m instead of x to convey that

¹This choice is contrary to the spin-statistics theorem; but that does not matter for our purposes, as the latter pre-supposes Lorentz invariance.

the configuration consists of m x -particles, and likewise y^n instead of y . We call $(\mathbb{R}^3)^m$ the m -particle sector of \mathcal{Q}_x and $(\mathbb{R}^3)^m \times (\mathbb{R}^3)^n$ the (m, n) -particle sector of $\mathcal{Q}_x \times \mathcal{Q}_y$. Likewise, we say (m, n) -particle sector of \mathcal{H} (or of Ψ , or of ψ) and write $\mathcal{H}^{(m, n)}$ (or $\Psi^{(m, n)}$ or $\psi^{(m, n)}$) for $S_- L^2(\mathbb{R}^3, \mathbb{C})^{\otimes m} \otimes S_+ L^2(\mathbb{R}^3, \mathbb{C})^{\otimes n}$, respectively for the projection of Ψ to that subspace, and for the restriction of ψ to $(\mathbb{R}^3)^m \times (\mathbb{R}^3)^n$. The $\psi^{(m, n)}$ function is anti-symmetric in the x variables and symmetric in the y variables.

The spaces $\mathcal{Q}_x, \mathcal{Q}_y$ are equipped with the volume measure

$$\mu(S) = \sum_{n=0}^{\infty} \text{vol}_{3n}(S \cap \mathcal{Q}_n) \quad \text{for } S \subseteq \mathcal{Q}_x. \quad (7)$$

The inner product in \mathcal{H} is then given by

$$\langle \psi | \phi \rangle = \int_{\mathcal{Q}_x} \mu(dx) \int_{\mathcal{Q}_y} \mu(dy) \psi^*(x, y) \phi(x, y) \quad (8)$$

$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \left\langle \psi^{(m, n)} \middle| \phi^{(m, n)} \right\rangle_{L^2(\mathbb{R}^{3m+3n})}. \quad (9)$$

2.1.1 Original Hamiltonian

As our example of a (non-relativistic) Hamiltonian H_{orig} , we take

$$\begin{aligned} (H_{\text{orig}}\psi)(x^m, y^n) &= -\frac{\hbar^2}{2m_x} \sum_{i=1}^m \nabla_{\mathbf{x}_i}^2 \psi(x^m, y^n) - \frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi(x^m, y^n) \\ &\quad + nE_0 \psi(x^m, y^n) \\ &\quad + g\sqrt{n+1} \sum_{i=1}^m \psi(x^m, (y^n, \mathbf{x}_i)) \\ &\quad + \frac{g}{\sqrt{n}} \sum_{i=1}^m \sum_{j=1}^n \delta^3(\mathbf{x}_i - \mathbf{y}_j) \psi(x^m, y^n \setminus \mathbf{y}_j), \end{aligned} \quad (10)$$

using the notation δ^3 for the 3-dimensional Dirac delta function and

$$y^n \setminus \mathbf{y}_j = (\mathbf{y}_1, \dots, \mathbf{y}_{j-1}, \mathbf{y}_{j+1}, \dots, \mathbf{y}_n) \quad (11)$$

for the configuration of $n-1$ y -particles with the j -th particle removed; E_0 is the energy that must be expended for creating a y -particle (the “ y rest energy”), and $g \in \mathbb{R}$ is a coupling constant (i.e., the “charge” of an x -particle). The first term in (10) is the free fermion Hamiltonian $H_x \psi$, the second and third terms are the free boson Hamiltonian $H_y \psi$, and the third and fourth line together are the interaction Hamiltonian $H_{\text{inter}} \psi$ responsible for the creation and annihilation of y -particles. In terms of creation and

annihilation operators,

$$H_x = \frac{\hbar^2}{2m_x} \int d^3 \mathbf{q} \nabla a_x^\dagger(\mathbf{q}) \nabla a_x(\mathbf{q}) \quad (12)$$

$$H_y = \frac{\hbar^2}{2m_y} \int d^3 \mathbf{q} \nabla a_y^\dagger(\mathbf{q}) \nabla a_y(\mathbf{q}) + E_0 \int d^3 \mathbf{q} a_y^\dagger(\mathbf{q}) a_y(\mathbf{q}) \quad (13)$$

$$H_{\text{inter}} = g \int d^3 \mathbf{q} a_x^\dagger(\mathbf{q}) (a_y(\mathbf{q}) + a_y^\dagger(\mathbf{q})) a_x(\mathbf{q}) \quad (14)$$

with † denoting the adjoint operator, and $a_{x,y}(\mathbf{q})$ the annihilation operators for an x, y -particle at location \mathbf{q} in position space, formally defined by

$$(a_x(\mathbf{q}) \psi)(x^m, y^n) = \sqrt{m+1} \psi((x^m, \mathbf{q}), y^n) \quad (15)$$

$$(a_x^\dagger(\mathbf{q}) \psi)(x^m, y^n) = \frac{1}{\sqrt{m}} \sum_{i=1}^m (-1)^i \delta^3(\mathbf{x}_i - \mathbf{q}) \psi(x^m \setminus \mathbf{x}_i, y^n), \quad (16)$$

$$(a_y(\mathbf{q}) \psi)(x^m, y^n) = \sqrt{n+1} \psi(x^m, (y^n, \mathbf{q})) \quad (17)$$

$$(a_y^\dagger(\mathbf{q}) \psi)(x^m, y^n) = \frac{1}{\sqrt{n}} \sum_{j=1}^n \delta^3(\mathbf{y}_j - \mathbf{q}) \psi(x^m, y^n \setminus \mathbf{y}_j). \quad (18)$$

The combinatorial factors $\sqrt{m+1}$ and $m^{-1/2}$ arise from the fact that every configuration of m x -particles occurs in $m!$ different permutations. Since the operators $a_{x,y}(\mathbf{q})$ contain the point evaluation of functions, they can actually be defined rigorously on a dense subspace of \mathcal{H} , while their adjoints are undefined for any nonzero ψ .

Model 1 is not Galilean covariant but a variant that is can be set up; it is defined, along with a version using IBCs, in [17].

2.1.2 UV Divergence of the Original Hamiltonian

The original Hamiltonian H_{orig} as defined in (10) above is UV divergent and thus ill defined. The source of the difficulty is the delta function in the last line of (10): Since a delta function is not a square-integrable function, the right-hand side of (10) does not lie in \mathcal{H} for any choice of ψ ; thus, (10) does not define an operator in \mathcal{H} . It can also be pointed out that the delta function δ^3 (which plays the role in (10) of the wave function of a newly created y -particle) is a state of infinite energy,

$$\text{formally} \quad \left\langle \delta^3 \left| \left(-\frac{\hbar^2}{2m_y} \nabla^2 \right) \right| \delta^3 \right\rangle = \int_{\mathbb{R}^3} d^3 \mathbf{k} \frac{(\hbar \mathbf{k})^2}{2m_y} = \infty. \quad (19)$$

The standard procedure for obtaining a well-defined Hamiltonian (UV cut-off) is to

replace the delta function by a square-integrable function $\varphi : \mathbb{R}^3 \rightarrow \mathbb{C}$, yielding

$$\begin{aligned}
(H_{\text{cutoff}}\psi)(x^m, y^n) &= -\frac{\hbar^2}{2m_x} \sum_{i=1}^m \nabla_{\mathbf{x}_i}^2 \psi(x^m, y^n) - \frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi(x^m, y^n) \\
&\quad + nE_0 \psi(x^m, y^n) \\
&\quad + g\sqrt{n+1} \sum_{i=1}^m \int_{\mathbb{R}^3} d^3\mathbf{y} \varphi^*(\mathbf{x}_i - \mathbf{y}) \psi(x^m, (y^n, \mathbf{y})) \\
&\quad + \frac{g}{\sqrt{n}} \sum_{i=1}^m \sum_{j=1}^n \varphi(\mathbf{x}_i - \mathbf{y}_j) \psi(x^m, y^n \setminus \mathbf{y}_j), \tag{20}
\end{aligned}$$

which amounts to saying that an x -particle has an extended charge distribution with density function φ (if φ is real-valued). Equivalently, the interaction Hamiltonian is replaced by

$$H_{\text{inter,cutoff}} = g \int d^3\mathbf{q} a_x^\dagger(\mathbf{q}) (a_{y,\varphi}(\mathbf{q}) + a_{y,\varphi}^\dagger(\mathbf{q})) a_x(\mathbf{q}), \tag{21}$$

where

$$(a_{y,\varphi}(\mathbf{q}) \psi)(x^m, y^n) = \sqrt{n+1} \int_{\mathbb{R}^3} d^3\mathbf{y} \varphi^*(\mathbf{q} - \mathbf{y}) \psi(x^m, (y^n, \mathbf{y})) \tag{22}$$

$$(a_{y,\varphi}^\dagger(\mathbf{q}) \psi)(x^m, y^n) = \frac{1}{\sqrt{n}} \sum_{j=1}^n \varphi(\mathbf{y}_j - \mathbf{q}) \psi(x^m, y^n \setminus \mathbf{y}_j). \tag{23}$$

2.2 Simplified Version: Model 2

In Model 2, there is only one x -particle, and it is fixed at the origin. The only dynamical (and quantized) degrees of freedom reside in the y -particles; such models were considered by van Hove [19, 3], and they tend to arise in the limit $m_x \rightarrow \infty$. Specifically, we take the configuration space of Model 2 to be the set

$$\mathcal{Q} = \mathcal{Q}_y = \bigcup_{n=0}^{\infty} \mathcal{Q}_y^{(n)} = \bigcup_{n=0}^{\infty} (\mathbb{R}^3 \setminus \{\mathbf{0}\})^n, \tag{24}$$

where $\mathbf{0}$ denotes the origin in \mathbb{R}^3 ; a configuration is denoted by $y^n = (\mathbf{y}_1, \dots, \mathbf{y}_n)$. Note that we exclude the possibility that any y -particle can be at the location of the x -particle (i.e., the origin), but we do not exclude the possibility that two y -particles can be at the same location because for the purposes of this model, in which the y -particles do not interact, there is no need to exclude such configurations.

Correspondingly, we take the Hilbert space to be the bosonic Fock space

$$\mathcal{H} = \mathcal{F}^+ = \bigoplus_{n=0}^{\infty} S_+ L^2(\mathbb{R}^3)^{\otimes n}. \tag{25}$$

Since for the definition of the Hilbert space it plays no role whether the origin is excluded or not, elements $\psi \in \mathcal{H}$ can be regarded as complex-valued functions on \mathcal{Q} that are permutation-symmetric in every sector; thus, $\mathcal{H} \subset L^2(\mathcal{Q})$, where \mathcal{Q} is thought of as equipped with the measure μ defined in the same way as in (7) ($L^2(\mathcal{Q})$ contains also non-symmetric functions). The “original” Hamiltonian is now a simplified version of (10):

$$\begin{aligned} (H_{\text{orig}}\psi)(y^n) &= -\frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi(y^n) + nE_0\psi(y^n) \\ &\quad + g\sqrt{n+1} \psi(y^n, \mathbf{0}) \\ &\quad + \frac{g}{\sqrt{n}} \sum_{j=1}^n \delta^3(\mathbf{y}_j) \psi(y^n \setminus \mathbf{y}_j), \end{aligned} \quad (26)$$

Also this Hamiltonian is UV divergent. In the following, we will sometimes find it useful to write $\psi^{(n)}(y^n)$ instead of $\psi(y^n)$ in order to emphasize which sector of ψ is being used.

3 Interior–Boundary Condition and Corresponding Hamiltonian for the Two Models

For Model 1 and Model 2, we describe the IBC and the Hamiltonian H_{IBC} . We also explain why H_{IBC} is a reasonable interpretation of the formula for H_{orig} . We begin with the simpler scenario of Model 2.

3.1 IBC for Model 2

Let \mathbb{S}^2 denote the unit sphere in \mathbb{R}^3 . The IBC demands the following: For every $\boldsymbol{\omega} \in \mathbb{S}^2$, $n \in \{0, 1, 2, \dots\}$, $y^n \in (\mathbb{R}^3 \setminus \{\mathbf{0}\})^n$,

$$\lim_{r \searrow 0} \left(r \psi^{(n+1)}(y^n, r\boldsymbol{\omega}) \right) = -\frac{g m_y}{2\pi \hbar^2 \sqrt{n+1}} \psi^{(n)}(y^n). \quad (27)$$

The IBC is a condition on the wave function ψ at or near the “boundary” of configuration space; the relevant boundary $\partial \mathcal{Q}_y^{(n)}$ of $\mathcal{Q}_y^{(n)}$ is

$$\partial \mathcal{Q}_y^{(n)} = \bigcup_{j=1}^n (\mathbb{R}^3)^{j-1} \times \{\mathbf{0}\} \times (\mathbb{R}^3)^{n-j}. \quad (28)$$

That is, the boundary consists of those configurations at which one of the y -particles collides with the x -particle. Due to the permutation symmetry of $\psi^{(n+1)}$, we can assume without loss of generality that it is the $n+1$ -st variable, \mathbf{y}_{n+1} , that approaches $\mathbf{0}$. The name “interior–boundary condition” reflects the fact that (27) relates the values (or

limits) of ψ on the boundary $\partial\mathcal{Q}_y$ to values of ψ in the interior of configuration space \mathcal{Q} (namely, in the interior of a different sector corresponding to a lesser number of y -particles).

The IBC (27) allows in particular that $\psi(y^n, r\omega)$ diverges like $1/r$ as $r \rightarrow 0$. In fact, it requires that ψ so diverges whenever the right-hand side of (27) is nonzero.² By permutation symmetry, $\psi(y^n)$ diverges as *any* \mathbf{y}_j approaches $\mathbf{0}$.

On wave functions ψ satisfying the IBC (27), the Hamiltonian $H = H_{IBC}$ is defined by

$$\begin{aligned} (H_{IBC}\psi)^{(n)}(y^n) &= -\frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi^{(n)}(y^n) + nE_0 \psi^{(n)}(y^n) \\ &\quad + \frac{g\sqrt{n+1}}{4\pi} \int_{\mathbb{S}^2} d^2\omega \lim_{r \searrow 0} \frac{\partial}{\partial r} \left(r\psi^{(n+1)}(y^n, r\omega) \right) \\ &\quad + \frac{g}{\sqrt{n}} \sum_{j=1}^n \delta^3(\mathbf{y}_j) \psi^{(n-1)}(y^n \setminus \mathbf{y}_j). \end{aligned} \tag{29}$$

This equation differs from the expression (26) for H_{orig} only in the second line, where $\psi(y^n, \mathbf{0})$ has been replaced by a more complicated expression involving the behavior of ψ near the configuration $(y^n, \mathbf{0})$; after all, ψ diverges at this configuration by virtue of the IBC, so the expression $\psi(y^n, \mathbf{0})$ does not make sense.

In view of the delta function appearing in (29), it may seem unlikely that such a Hamiltonian can be well defined. However, Theorem 1 in Section 3.2 below shows that in fact it is well defined. It turns out that the last line in (29) always gets canceled by contributions to the first line, which may contain delta functions because we now allow wave functions that diverge like $1/r = 1/|\mathbf{y}_j|$, and the Laplacian of $1/r$ is $4\pi\delta^3$ (as readers may remember from electrostatics, where $1/r$ occurs as the Coulomb potential ϕ generated by a point charge, satisfying the Poisson equation $\Delta\phi = 4\pi\rho$ with charge density ρ). As a consequence of this cancelation, $H_{IBC}\psi$ is a square-integrable function for ψ satisfying the IBC. See also Remark 6 in Section 3.3 below for further discussion.

Let us point out a connection between the second line of (29), the line that differed from the original Hamiltonian (26), and the corresponding line in (26). Think of $\psi(y^n, r\omega)$ as a function of r ; as $r \rightarrow 0$, it can be expanded in the form $\psi(y^n, r\omega) = a/r + b + O(r)$ with complex coefficients a, b ; then

$$\frac{\partial}{\partial r}(r\psi) = b + O(r), \tag{30}$$

²This divergence is to be expected if we keep in mind that $|\psi|^2$ represents probability density and note that for the inward radial flow in \mathbb{R}^3 , i.e., for the dynamical system defined by the ODE $\dot{\mathbf{x}} = -\mathbf{x}/|\mathbf{x}|$, the stationary density is $1/r^2 = 1/|\mathbf{x}|^2$. To see this, note that if we squeeze a spherical shell of radius r_1 and thickness dr to a shell with smaller radius r_2 and equal thickness dr then its volume goes down (and thus, if its probability content is conserved, its density goes up) by a factor of $(r_1/r_2)^2$. That is why to expect $|\psi|^2 \sim 1/r^2$ and thus $\psi \sim 1/r$ as $r \rightarrow 0$.

which yields b in the limit $r \rightarrow 0$, and if ψ did not diverge as $r \rightarrow 0$, this would be exactly the value $b = \lim_{r \searrow 0} \psi(y^n, r\omega) = \psi(y^n, \mathbf{0})$ occurring in (26) in the second line. So, (29) is really quite similar to (26).

The Hamiltonian H_{IBC} is *not* the sum of two self-adjoint operators, the free Hamiltonian and an interaction Hamiltonian. That is because the free Hamiltonian is defined on a different domain than H_{IBC} , containing wave functions that do not satisfy the IBC and do not diverge on the diagonal. It is the action of the Laplacian on functions that diverge on the diagonal that leads to delta functions and thus makes the last line of (29) possible, and it is only in conjunction with the IBC that the Hamiltonian (29) leads to conservation of probability.

Indeed, in order to understand why the IBC (27) was chosen this way, and how it works together with the formula (29) for the Hamiltonian, it is illuminating to calculate the balance equation for $|\psi|^2$ and check that $|\psi|^2$ is conserved. We go through such a calculation in the next section.

3.2 Self-Adjointness and Conservation of Probability

Theorem 1. [9] *On a certain dense subspace \mathcal{D}_{IBC} of $\mathcal{H} = \mathcal{F}^+$, the elements of which satisfy the IBC (27), the operator H_{IBC} given by (29) is well-defined and self-adjoint. If $E_0 > 0$, then H_{IBC} is positive.*

The relevance of this theorem is that it provides certainty that H_{IBC} is not afflicted by UV divergence. We give here a calculation checking on a non-rigorous level that probability is conserved. Using the symbol

$$\mathbf{j}_{\mathbf{y}_j} = \mathbf{j}_{\mathbf{y}_j}(y^n) = \frac{\hbar}{m_y} \text{Im} \psi^* \nabla_{\mathbf{y}_j} \psi \quad (31)$$

for the usual probability current, we obtain from (29) that, at any configuration y^n (without any y -particle at the origin),

$$\begin{aligned} \frac{\partial |\psi(y^n)|^2}{\partial t} &= - \sum_{j=1}^n \nabla_{\mathbf{y}_j} \cdot \mathbf{j}_{\mathbf{y}_j} \\ &\quad + \frac{g\sqrt{n+1}}{2\pi\hbar} \text{Im} \psi^*(y^n) \int_{\mathbb{S}^2} d^2\omega \lim_{r \searrow 0} \frac{\partial}{\partial r} \left(r \psi(y^n, r\omega) \right). \end{aligned} \quad (32)$$

The last line can be re-written, using the IBC (27), as

$$- \frac{g\sqrt{n+1}}{2\pi\hbar} \text{Im} \frac{2\pi\hbar^2\sqrt{n+1}}{g m_y} \lim_{r \searrow 0} r \psi^*(y^n, r\omega) \int_{\mathbb{S}^2} d^2\omega \lim_{r \searrow 0} \frac{\partial}{\partial r} \left(r \psi(y^n, r\omega) \right) \quad (33)$$

$$= -(n+1) \lim_{r \searrow 0} r^2 \int_{\mathbb{S}^2} d^2\omega \frac{\hbar}{m_y} \text{Im} \psi^*(y^n, r\omega) \frac{\partial}{\partial r} \psi(y^n, r\omega), \quad (34)$$

using that $\partial_r(r\psi) = \psi + r\partial_r\psi$ and $\text{Im}(r|\psi|^2) = 0$. Thus,

$$\frac{\partial|\psi(y^n)|^2}{\partial t} = -\sum_{j=1}^n \nabla_{\mathbf{y}_j} \cdot \mathbf{j}_{\mathbf{y}_j} - (n+1) \lim_{r \searrow 0} r^2 \int_{\mathbb{S}^2} d^2\boldsymbol{\omega} \boldsymbol{\omega} \cdot \mathbf{j}_{\mathbf{y}_{n+1}}(y^n, r\boldsymbol{\omega}). \quad (35)$$

This equation possesses a simple interpretation: $-r^2$ times the integral is just the flux of probability current toward the origin across the sphere of radius r in the coordinate space of \mathbf{y}_{n+1} ; the limit of that as $r \rightarrow 0$ is the current of probability into the origin in the coordinate space of \mathbf{y}_{n+1} ; summing over all y -particles would yield, due to the bosonic symmetry of ψ , $n+1$ equal terms; thus, the second summand on the right-hand side of (35) is the total flux of probability into the boundary configurations obtained from y^n by adding one y -particle at the origin. That is, the balance equation (35) asserts that the probability density $|\psi|^2$ changes in two ways, due to transport of probability in the n -particle sector and by increasing at just the rate at which probability disappears on the $(n+1)$ -particle sector by flowing into the boundary $\partial\mathcal{Q}_y^{(n+1)}$. Therefore, total probability is conserved.

3.3 Remarks

1. *Comparison to Bethe–Peierls boundary condition.* The IBC (46) has some parallels to the Bethe–Peierls boundary condition [2], which reads for a wave function $\psi \in L^2(\mathbb{R}^3, \mathbb{C})$:

$$\lim_{r \searrow 0} \left(\alpha + \frac{\partial}{\partial r} \right) (r\psi(r\boldsymbol{\omega})) = 0 \quad (36)$$

with given constant $\alpha \in \mathbb{R}$. This condition is used for giving precise meaning to a Schrödinger equation for $\psi : \mathbb{R}^3 \rightarrow \mathbb{C}$ with a Dirac delta function as the potential,

$$H = -\frac{\hbar^2}{2m} \Delta + g \delta^3(\mathbf{x}), \quad (37)$$

a kind of interaction known as a *point interaction* [1]. Like our IBCs (27), (43), (46), the Bethe–Peierls boundary condition (36) concerns the “boundary” at $r = 0$. However, in contrast to the IBC, which connects two sectors of \mathcal{Q} , the Bethe–Peierls boundary condition involves only one sector, as the wave function ψ is defined on \mathbb{R}^3 . Also, the Bethe–Peierls boundary condition implies zero current into $r = 0$ (see, e.g., [16] for more detail), whereas the IBC leads to a nonzero current into the boundary.

2. *Comparison to vertex conditions in networks.* An example of a known boundary condition leading to nonzero current into the boundary is provided by the vertex conditions for quantum mechanics on networks (see, e.g., [8] and references therein). A network, or graph, consists of several 1-dimensional spaces (i.e., intervals) called edges, glued together at their end points called vertices. The wave function is a (say, complex-valued) function on the network (i.e., on the union of

the edges), and the Hamiltonian is given by the Laplace operator on each edge, along with boundary conditions for the end points of the edges, also called vertex conditions. The vertex conditions are related to the fact that, since no positive amount of probability can be located at a vertex, all of the probability current into the vertex must be compensated by a current out of the vertex; that is, for each vertex v , the sum of the currents along all edges e connected to v (pointing away from v) must vanish,

$$\sum_e j_e(v) = 0. \quad (38)$$

While Dirichlet or Neumann boundary condition at every end point of every edge would lead to $j_e(v) = 0$ for all v and e , it is also possible to impose vertex conditions on ψ that allow nonzero flow of probability from one edge across a vertex to another edge, the simplest one being the conjunction of

$$\lim_{x \rightarrow v \text{ along } e} \psi(x) = \lim_{x \rightarrow v \text{ along } e'} \psi(x), \quad (39)$$

i.e., that ψ is continuous at vertices, and

$$\sum_e \partial_e \psi(v) = \alpha \psi(v), \quad (40)$$

where $\alpha \in \mathbb{R}$ is a given constant and $\partial_e \psi(v)$ means the derivative of ψ along the edge e , taken at v .

To draw parallels between (40) and IBCs, we may compare the edges of a network to the sectors of the configuration spaces considered in this paper; let us call both the “blocks” of the space. Of course, the edges of a graph have equal dimension while the sectors of our \mathcal{Q} have different dimension. We may note that in both situations the probability loss in one block is compensated by a probability gain in others. Also, the condition of continuity (39) is a relation between the boundary value in one block and a value in another, but in contrast to an IBC the latter is also a boundary value; that is, in analogy to the terminology “interior–boundary condition,” (39) is a “boundary–boundary condition.”

3. *Combinatorial factors.* As remarked at the end of Section 2.1.1, the combinatorial factors \sqrt{n} and $\sqrt{n+1}$ that appear in the Hamiltonian arise from the fact that we use *ordered* configurations $(\mathbf{y}_1, \dots, \mathbf{y}_n)$ although in nature configurations are *unordered*, as in $\{\mathbf{y}_1, \dots, \mathbf{y}_n\}$. This is also true of the IBC (27) and the associated Hamiltonian (29). If we used unordered configurations, which leads to topologically non-trivial configuration spaces (see, e.g., [13, 6]), these factors would not appear.
4. *Neumann-type IBC.* Two well known types of boundary conditions are Dirichlet boundary conditions,

$$\psi \Big|_{\partial \mathcal{Q}} = 0, \quad (41)$$

and Neumann boundary conditions,

$$\left. \frac{\partial \psi}{\partial n} \right|_{\partial \mathcal{Q}} = 0, \quad (42)$$

with n the normal vector on the boundary hypersurface. While the IBC (27) resembles the Dirichlet type in that it involves the *values* of ψ (or rather, $r\psi$) on the boundary, one can as well set up a different IBC that resembles the Neumann type in that it involves the *normal derivative* of ψ (or rather, $r\psi$). Here, $r = 0$ plays the role of the boundary, and the radial direction plays the role of the normal to the boundary. The *Neumann-type IBC* asserts that for any $n \in \{0, 1, 2, \dots\}$, any configuration $y^n \in (\mathbb{R}^3 \setminus \{\mathbf{0}\})^n$, and any $\boldsymbol{\omega} \in \mathbb{S}^2$,

$$\lim_{r \searrow 0} \frac{\partial}{\partial r} (r\psi(y^n, r\boldsymbol{\omega})) = \frac{g m_y}{2\pi \hbar^2 \sqrt{n+1}} \psi(y^n). \quad (43)$$

Also this IBC typically leads to $\psi(y^n, r\boldsymbol{\omega})$ diverging like $1/r$ as $r \rightarrow 0$.

On wave functions ψ satisfying the IBC (43), the Hamiltonian $H = H_{IBC}$ is defined by

$$\begin{aligned} (H\psi)(y^n) = & -\frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi(y^n) + nE_0 \psi(y^n) \\ & + \frac{g\sqrt{n+1}}{4\pi} \int_{\mathbb{S}^2} d^2\boldsymbol{\omega} \lim_{r \searrow 0} r\psi(y^n, r\boldsymbol{\omega}) \\ & + \frac{\hbar^2}{2m_y} \sum_{j=1}^n \delta^3(\mathbf{y}_j) \int_{\mathbb{S}^2} d^2\boldsymbol{\omega} \lim_{r \searrow 0} r\psi(y^n \setminus \mathbf{y}_j, r\boldsymbol{\omega}). \end{aligned} \quad (44)$$

This equation differs from (29) (for the Dirichlet case) in the second line, which no longer involves a derivative, and in the last line, which we will discuss further in Remark 6 below.

While (43) and (44) together define a different time evolution for ψ than (27) and (29), Equation (35) is still true and guarantees that the amount of probability lost on the $n+1$ -sector of \mathcal{Q} due to probability flux into the boundary is added on the n -sector. This fact suggests that also (43) and (44) define a self-adjoint operator.

5. *Robin-type IBC.* A Robin boundary condition is one of the form

$$\left(\alpha\psi + \beta \frac{\partial \psi}{\partial n} \right) \Big|_{\partial \mathcal{Q}} = 0 \quad (45)$$

with given constants α and β . An IBC of an analogous form can be set up as follows: for any $n \in \{0, 1, 2, \dots\}$, any configuration $y^n = (\mathbf{y}_1, \dots, \mathbf{y}_n) \in (\mathbb{R}^3 \setminus \{\mathbf{0}\})^n$

of y -particles, and any $\boldsymbol{\omega} \in \mathbb{S}^2$,

$$\lim_{r \searrow 0} \left(\alpha + \beta \frac{\partial}{\partial r} \right) \left(r \psi(y^n, r \boldsymbol{\omega}) \right) = \frac{2m_y}{\hbar^2 \sqrt{n+1}} \psi(y^n), \quad (46)$$

where $(\alpha, \beta) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ are constants. Also this condition typically leads to ψ that diverge like $1/r$ as $r \rightarrow 0$. The Dirichlet-type condition (27) is included in this scheme for $\alpha = -4\pi/g, \beta = 0$, while the Neumann-type condition (43) is included for $\alpha = 0, \beta = 4\pi/g$.

The associated Hamiltonian $H = H_{IBC}$ is given by

$$\begin{aligned} H\psi(y^n) = & -\frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi(y^n) + nE_0 \psi(y^n) \\ & + \sqrt{n+1} \int_{\mathbb{S}^2} d^2\boldsymbol{\omega} \lim_{r \searrow 0} \left(\gamma + \delta \frac{\partial}{\partial r} \right) \left(r \psi(y^n, r \boldsymbol{\omega}) \right) \\ & + \frac{\hbar^2}{2m_y} \sum_{j=1}^n \delta^3(\mathbf{y}_j) \int_{\mathbb{S}^2} d^2\boldsymbol{\omega} \lim_{r \searrow 0} r \psi(y^n \setminus \mathbf{y}_j, r \boldsymbol{\omega}), \end{aligned} \quad (47)$$

where the constants $\gamma, \delta \in \mathbb{C}$ satisfy

$$\alpha^* \gamma \in \mathbb{R} \quad (48)$$

$$\beta^* \delta \in \mathbb{R} \quad (49)$$

$$\alpha^* \delta - \gamma^* \beta = -1. \quad (50)$$

It should always be obvious when the symbol δ means the constant $\delta \in \mathbb{C}$ and when the Dirac delta function. Note that for $\gamma = 0, \delta = g/4\pi$, the expression (47) for the Hamiltonian agrees with (29), while for $\gamma = g/4\pi, \delta = 0$ it reduces to (44).

On a non-rigorous level, the conservation of probability (i.e., self-adjointness of the Hamiltonian (47)) can be checked by means of a calculation similar to the one in Section 3.2 above and to the one in Section 4.3 below. The self-adjointness breaks down (already on the non-rigorous level) if we relax the conditions (48)–(50).

6. *Dirac delta function terms in H .* Here is a reason for thinking that, among the many different IBCs that are mathematically possible corresponding to different choices of the constants $\alpha, \beta, \gamma, \delta$, only the Dirichlet-type IBC (27), corresponding to $\alpha = -4\pi/g, \beta = 0 = \gamma$, and $\delta = g/4\pi$, is physically relevant as a replacement of the original (UV divergent) Hamiltonian (26): It is the only choice that leads to a term in H_{IBC} that reproduces the Dirac delta function terms in H_{orig} , i.e., for which the last line of (47) agrees with the last line of (26). That is because the Dirichlet case is the only case in which the last line of (47) can be expressed in terms of $\psi^{(n-1)}$.

And the last line of (47) is dictated by the condition that $H\psi$ has to be an L^2 function and thus cannot contain contributions that are Dirac delta functions. Indeed, since for any $\alpha, \beta, \gamma, \delta$, the wave function $\psi^{(n)}$ diverges at the boundary like $1/r$, the Laplacian in the Hamiltonian always yields a distribution of the form

$$-\sum_j \nabla_{\mathbf{y}_j}^2 \psi^{(n)} = -\sum_j \delta^3(\mathbf{y}_j) f(y^n \setminus \mathbf{y}_j) + g(y^n) \quad (51)$$

with some functions f and g ; so the Dirac delta contributions need to be canceled, which leads to the last line of (47).

7. *Positivity.* Another reason for thinking that the Dirichlet-type IBC (rather than, say, Neumann-type) is the physically relevant choice may be that H_{IBC} for a Dirichlet-type IBC is positive, as mentioned in Theorem 1 in Section 3.2. Generally speaking, the IBC approach neither requires nor guarantees that Hamiltonians are bounded from below. Presently, we do not know for which other choices of $\alpha, \beta, \gamma, \delta$ the Hamiltonian will be positive, but we see reason to believe that, in the variant of the equations appropriate for Model 1, the Neumann-type IBC leads to a Hamiltonian that is not bounded from below. Further considerations about physical reasonableness of H_{IBC} can be found in Sections 3.5 and 3.6 below.
8. *Bohmian trajectories.* There is a natural way of defining Bohmian trajectories for the models described in this paper; we describe this in detail elsewhere [5]. The Bohmian configuration Q_t follows a Markov jump process in configuration space that is $|\psi_t|^2$ -distributed at every time t . The process has finitely many jumps in every finite time interval and moves deterministically in-between according to Bohm's equation of motion. In our Models 1 and 2, the jumps correspond to the creation or annihilation of a particle. The jumps to a lower sector (particle annihilation) occur whenever a y -particle hits an x -particle; in that event, the y -particle gets deleted from Q_t . While the jumps to a lower sector are deterministic, the jumps to a higher sector (particle creation) are stochastic. They can occur at any configuration Q_t , with a rate depending on Q_t and ψ_t , and lead to a configuration with a new y -particle created at the location of an x -particle; the y -particle then moves in a random direction that is uniformly distributed over the sphere. Compared to previous models of particle creation and annihilation in Bohmian mechanics (see [18] and references therein) that involved a UV cut-off, the difference is that in Models 1 and 2, the y -particle gets created *at* (rather than *near*) an x -particle, and that annihilation is deterministic. The process is time-reversal invariant (notwithstanding that annihilation is deterministic and creation is stochastic).

3.4 IBC for Model 1

We now describe an IBC and the corresponding Hamiltonian for Model 1. The IBC demands that for any $m, n \in \{1, 2, \dots\}$, any configuration $x^m = (\mathbf{x}_1, \dots, \mathbf{x}_m) \in \mathbb{R}^{3m}$ of

x -particles, any configuration $y^n = (\mathbf{y}_1, \dots, \mathbf{y}_n) \in \mathbb{R}^{3n}$ of y -particles with $x^m \cap y^n = \emptyset$ (i.e., $\mathbf{x}_i \neq \mathbf{y}_j$ for all i, j), any $i = 1, \dots, m$, and any $j = 1, \dots, n$,

$$\lim_{(\mathbf{x}_i, \mathbf{y}_j) \rightarrow (\mathbf{x}, \mathbf{x})} |\mathbf{y}_j - \mathbf{x}_i| \psi(x^m, y^n) = \alpha_{n-1} \psi(\mathbf{x}_i = \mathbf{x}, \widehat{\mathbf{y}}_j), \quad (52)$$

where $\widehat{}$ denotes omission,

$$\alpha_{n-1} = -\frac{g}{2\pi\hbar^2\sqrt{n}} \frac{m_x m_y}{m_x + m_y}, \quad (53)$$

and $g \in \mathbb{R}$ is the same coupling constant as before.

The IBC is a condition on the wave function ψ near the *diagonal* Δ in configuration space $\mathcal{Q}_x \times \mathcal{Q}_y$, i.e., the set of “collision configurations,”

$$\Delta = \left\{ (x^m, y^n) \in \mathcal{Q}_x \times \mathcal{Q}_y : \mathbf{x}_i = \mathbf{y}_j \text{ for some } i, j \right\}. \quad (54)$$

If we regard the collision configurations in Δ as not admissible configurations then the configuration space is the set difference $\mathcal{Q} = (\mathcal{Q}_x \times \mathcal{Q}_y) \setminus \Delta$, and its “boundary” is $\partial\mathcal{Q} = \Delta$.

On wave functions ψ satisfying the IBC (52), the Hamiltonian $H = H_{IBC}$ is defined by

$$\begin{aligned} (H_{IBC}\psi)(x^m, y^n) &= -\frac{\hbar^2}{2m_x} \sum_{i=1}^m \nabla_{\mathbf{x}_i}^2 \psi(x^m, y^n) - \frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi(x^m, y^n) \\ &+ nE_0 \psi(x^m, y^n) \\ &+ \frac{g\sqrt{n+1}}{4\pi} \sum_{i=1}^m \int_{\mathbb{S}^2} d^2\omega \lim_{r \searrow 0} \frac{\partial}{\partial r} \left[r \psi \left(\mathbf{x}_i \rightarrow \mathbf{x}_i - \mu_x r \omega, \mathbf{y}_{n+1} \rightarrow \mathbf{x}_i + \mu_y r \omega \right) \right] \\ &+ \frac{g}{\sqrt{n}} \sum_{i=1}^m \sum_{j=1}^n \delta^3(\mathbf{x}_i - \mathbf{y}_j) \psi(x^m, y^n \setminus \mathbf{y}_j) \end{aligned} \quad (55)$$

with

$$\mu_x = \frac{m_y}{m_x + m_y} \text{ and } \mu_y = \frac{m_x}{m_x + m_y}. \quad (56)$$

We conjecture (and are working on a proof [10]) that H_{IBC} given by (55) defines a self-adjoint operator on a suitable dense subspace of $\mathcal{H} = \mathcal{F}^- \otimes \mathcal{F}^+$, the elements of which satisfy the IBC (52).

3.5 Ground State Energy and Effective Yukawa Potential

Elsewhere [9] we show that H_{IBC} as in (29) for Model 2 with Dirichlet-type IBC (27) possesses a non-degenerate ground state ψ_{\min} . It is given by

$$\psi_{\min}(\mathbf{y}_1, \dots, \mathbf{y}_n) = \mathcal{N} \frac{1}{\sqrt{n!}} \left(-\frac{gm_y}{2\pi\hbar^2} \right)^n \prod_{j=1}^n \frac{e^{-\sqrt{2m_y E_0} |\mathbf{y}_j|/\hbar}}{|\mathbf{y}_j|} \quad (57)$$

with normalization constant

$$\mathcal{N} = \exp\left(-\frac{g^2 m_y^2}{4\pi \hbar^3 \sqrt{2m_y E_0}}\right) \quad (58)$$

and eigenvalue

$$E_{\min} = \frac{g^2 m_y \sqrt{2m_y E_0}}{2\pi \hbar^3}. \quad (59)$$

That is, the state is a superposition of different numbers of y -particles, and in each sector all y -particles have the same wave function; so the x -particle at the origin is dressed with a cloud of y -particles. The probability distribution of the number n of y -particles is a Poisson distribution with mean value

$$\langle n \rangle_{\psi_{\min}} = \frac{g^2 m_y^2}{2\pi \hbar^3 \sqrt{2m_y E_0}}. \quad (60)$$

We claim further that in Model 1, in which the x -particles interact by exchanging y -particles, the x -particles effectively interact through a Yukawa potential; this in fact agrees with the result of Yukawa's original reasoning [20], see below. A simple way of computing the effective interaction potential is to consider (as "Model 2b") N x -particles fixed at $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^3$ and to find the ground state energy. To this end, consider wave functions of y -configurations that simultaneously satisfy N IBCs,

$$\lim_{r \searrow 0} \left(r \psi^{(n+1)}(y^n, \mathbf{x}_i + r\boldsymbol{\omega}) \right) = -\frac{g m_y}{2\pi \hbar^2 \sqrt{n+1}} \psi^{(n)}(y^n) \quad (61)$$

for every $i = 1, \dots, N$, $\boldsymbol{\omega} \in \mathbb{S}^2$, $n \in \{0, 1, 2, \dots\}$, and $y^n \in (\mathbb{R}^3 \setminus \{\mathbf{x}_1, \dots, \mathbf{x}_N\})^n$. The corresponding Hamiltonian reads

$$\begin{aligned} (H\psi)^{(n)}(y^n) &= -\frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi^{(n)}(y^n) + n E_0 \psi^{(n)}(y^n) \\ &+ \frac{g \sqrt{n+1}}{4\pi} \sum_{i=1}^N \int_{\mathbb{S}^2} d^2 \boldsymbol{\omega} \lim_{r \searrow 0} \frac{\partial}{\partial r} \left(r \psi^{(n+1)}(y^n, \mathbf{x}_i + r\boldsymbol{\omega}) \right) \\ &+ \frac{g}{\sqrt{n}} \sum_{i=1}^N \sum_{j=1}^n \delta^3(\mathbf{y}_j - \mathbf{x}_i) \psi^{(n-1)}(y^n \setminus \mathbf{y}_j). \end{aligned} \quad (62)$$

For $E_0 > 0$, the ground state is

$$\psi_{\min}(\mathbf{y}_1, \dots, \mathbf{y}_n) = c_n \prod_{j=1}^n \sum_{i=1}^N \frac{e^{-\sqrt{2m_y E_0} |\mathbf{y}_j - \mathbf{x}_i|/\hbar}}{|\mathbf{y}_j - \mathbf{x}_i|} \quad (63)$$

with suitable factors c_n and eigenvalue

$$E_{\min} = \frac{g^2 m_y}{\pi \hbar^2} \left(\frac{N \sqrt{2m_y E_0}}{2\hbar} - \sum_{1 \leq i < j \leq N} \frac{e^{-\sqrt{2m_y E_0} |\mathbf{x}_i - \mathbf{x}_j|/\hbar}}{|\mathbf{x}_i - \mathbf{x}_j|} \right). \quad (64)$$

That is, the ground state energy of the y -particles, given the x -particles at $\mathbf{x}_1, \dots, \mathbf{x}_N$, is given by (64). Regarding this energy function of $\mathbf{x}_1, \dots, \mathbf{x}_N$ as an effective potential for the x -particles (which is appropriate when the x -particles move slowly), we see that x -particles effectively interact through an attractive Yukawa pair potential,

$$V(R) = \text{const.} - \frac{e^{-\lambda R}}{R} \quad (65)$$

with R the distance between two x -particles. If we take the energy needed to create a y -particle to be $E_0 = m_y c^2$, then

$$\lambda = \sqrt{2} \frac{m_y c}{\hbar}, \quad (66)$$

which is, up to the factor $\sqrt{2}$, the value originally obtained by Yukawa [20] considering the effective interaction of nucleons by exchange of pions. We expect that the factor $\sqrt{2}$ is owed to the non-relativistic nature of our model.

3.6 IBC Hamiltonians as a Limit of Removing the Cut-Off

If one introduces a UV cut-off into the UV divergent original Hamiltonian (26) of Model 2, it becomes the well-defined operator H_φ given by

$$\begin{aligned} H_\varphi \psi(y^n) = & -\frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi(y^n) + n E_0 \psi(y^n) \\ & + g \sqrt{n+1} \int_{\mathbb{R}^3} d^3 \mathbf{y} \varphi^*(\mathbf{y}) \psi(y^n, \mathbf{y}) \\ & + \frac{g}{\sqrt{n}} \sum_{j=1}^n \varphi(\mathbf{y}_j) \psi(y^n \setminus \mathbf{y}_j), \end{aligned} \quad (67)$$

analogous to (20) for Model 1. Here, the Dirac delta function δ^3 has been replaced by $\varphi : \mathbb{R}^3 \rightarrow \mathbb{C}$, a square-integrable function describing the charge density of the x -particle, and the limit $\varphi \rightarrow \delta^3$ would correspond to removing the UV cut-off. It is well known [19, 3] that, if $E_0 > 0$, there are numbers $E_\varphi \in \mathbb{R}$ such that the operator $H_\varphi - E_\varphi$ possesses a limit as $\varphi \rightarrow \delta^3$; let us call this limit, which is a self-adjoint operator, H_∞ . Since $E_\varphi \rightarrow \infty$ in this limit, H_φ tends to infinity in a sense, but this sense is harmless because two Hamiltonians that differ only by a multiple of the identity operator can be regarded as equivalent, as they generate the same time evolution (if we regard wave functions that differ only by a global phase factor as equivalent). So, in a relevant sense, the limit $\varphi \rightarrow \delta^3$ can indeed be taken, and H_∞ is the limiting Hamiltonian, which suggests regarding H_∞ as the “physically correct” Hamiltonian.

Theorem 2. [9] *For the Hamiltonian H_{IBC} of the Dirichlet type for Model 2, defined by (27) and (29),*

$$H_\infty = H_{IBC} + E_\infty \quad (68)$$

with the constant $E_\infty = g^2 \sqrt{E_0}/4\pi$.

On the one hand, this result lends further support to regarding H_{IBC} and the IBC approach as physically reasonable. On the other hand, the result provides a more direct representation of H_∞ than was available so far.

4 IBCs For Codimension-1 Boundaries

In Model 1 and Model 2, our examples for the application of IBCs to QFT, the boundary of each sector of configuration space was a subset of codimension 3, corresponding to an x -particle and a y -particle being at the same location. IBCs can also naturally be used for codimension-1 boundaries in configuration space, as we outline in this section. A simple example we describe elsewhere [16]. As far as we can see, the considerations in this section have no impact on avoiding the UV divergence without UV cut-off, but they form a natural framework, although not the most general one, for IBCs. Preliminary considerations in this direction were described in [18].

4.1 Configuration Space and Hilbert Space

We take the configuration space \mathcal{Q} to be a finite or countable union of disjoint manifolds with boundary, $\mathcal{Q} = \cup_n \mathcal{Q}^{(n)}$. (By definition, in a manifold with boundary, a neighborhood of an interior point looks like a piece of \mathbb{R}^d , while a neighborhood of a boundary point looks like a piece of a half-space in \mathbb{R}^d . In particular, the boundary has codimension 1, i.e., dimension $d - 1$. The boundary may be empty.) We write $\partial \mathcal{Q}^{(n)}$ for the boundary of $\mathcal{Q}^{(n)}$, $\partial \mathcal{Q} = \cup_n \partial \mathcal{Q}^{(n)}$, and $\mathcal{Q}^\circ = \mathcal{Q} \setminus \partial \mathcal{Q}$ for the interior of \mathcal{Q} . We take \mathcal{Q} to be equipped with a Riemann metric g_{ij} , which also defines a volume measure $\mu^{(n)}$ on $\mathcal{Q}^{(n)}$, and thus a measure μ on \mathcal{Q} , $\mu(S) = \sum_n \mu^{(n)}(S \cap \mathcal{Q}^{(n)})$; likewise, the metric defines a surface area measure λ on $\partial \mathcal{Q}$.

Wave functions can be complex-valued functions on \mathcal{Q} . However, we can also be more general and allow cross-sections of vector bundles. Readers unfamiliar with vector bundles may ignore this further generality and think of complex-valued wave functions. So, for every n , let $E^{(n)}$ be a *Hermitian vector bundle* over $\mathcal{Q}^{(n)}$ of finite rank $r_n = \dim_{\mathbb{C}} E_q^{(n)}$ (dimension of the fiber spaces), i.e., a complex vector bundle equipped with a positive definite Hermitian inner product $(\ , \)_q$ in every fiber $E_q^{(n)}$, $q \in \mathcal{Q}^{(n)}$, and a metric connection (i.e., a connection relative to which the inner product is parallel, or, equivalently, a connection such that the parallel transport it defines along any path from q to q' is a unitary isomorphism $E_q^{(n)} \rightarrow E_{q'}^{(n)}$). We write E for $\cup_n E^{(n)}$ and E_q for $E_q^{(n)}$ if $q \in \mathcal{Q}^{(n)}$. The wave function will be a cross-section of E , i.e., a mapping $\psi : \mathcal{Q} \rightarrow E$ such that $\psi(q) \in E_q$ for every $q \in \mathcal{Q}$.

The Hilbert space $\mathcal{H} = L^2(\mathcal{Q}, E, \mu)$ consists of the square-integrable cross-sections of E and is equipped with the inner product

$$\langle \psi | \phi \rangle = \int_{\mathcal{Q}} \mu(dq) (\psi(q), \phi(q))_q. \quad (69)$$

Note that $\int_{\mathcal{Q}}$ means the same as $\sum_n \int_{\mathcal{Q}^{(n)}}$, and that $\mathcal{H} = \oplus_n L^2(\mathcal{Q}^{(n)}, E^{(n)}, \mu^{(n)})$.

4.2 IBC and Hamiltonian

The IBC will be so constructed that the amount of probability per time that flows out of the boundary at $q' \in \partial\mathcal{Q}$ gets added to $|\psi|^2$ at an interior point

$$q = f(q') \quad (70)$$

in a different sector, $f : \partial\mathcal{Q} \rightarrow \mathcal{Q}^\circ$. We suppose that the derivative of f has full rank, i.e., that the image of f in $\mathcal{Q}^{(n)}$ does not have lower dimension than $\mathcal{Q}^{(n)}$; in particular, if $q' \in \partial\mathcal{Q}^{(n')}$ and $q = f(q') \in \mathcal{Q}^{(n)}$ then $\dim \mathcal{Q}^{(n)} \leq \dim \partial\mathcal{Q}^{(n')} = \dim \mathcal{Q}^{(n')} - 1$. Since many boundary points q' can be mapped to the same interior point q , the set of which will be denoted

$$f^{-1}(q) = \{q' \in \partial\mathcal{Q} : f(q') = q\}, \quad (71)$$

we will need to make use of a measure over $f^{-1}(q)$. The appropriate (unnormalized) measure for our purpose is

$$\nu_q(\cdot) = \text{weak-lim}_{dq \rightarrow \{q\}} \frac{\lambda(\cdot \cap f^{-1}(dq))}{\mu(dq)}. \quad (72)$$

For example, if $S = f^{-1}(q) \cap \partial\mathcal{Q}^{(n')}$ is a submanifold of $\partial\mathcal{Q}^{(n')}$ of dimension k and $\partial\mathcal{Q}^{(n')}$ has dimension ℓ , then the density of ν_q relative to the volume measure arising from the Riemann metric on S is

$$\left| \frac{\det(g_{\partial\mathcal{Q}^{(n')}}(e_i, e_j))_{i,j \leq \ell}}{\det(g_S(e_i, e_j))_{i,j \leq k} \det(g_{\mathcal{Q}^{(n)}}(df(e_i), df(e_j)))_{k < i, j \leq \ell}} \right|^{1/2}, \quad (73)$$

where $df : T_{q'}\partial\mathcal{Q} \rightarrow T_q\mathcal{Q}$ is the derivative of f , and e_i are any linearly independent vectors in $T_{q'}\partial\mathcal{Q}$ with the first k in $T_{q'}S$; the quantity (73) does not depend on the choice of e_i .³ In particular, if $f^{-1}(q)$ is a finite or countable set (say, f is a local diffeomorphism), then for any $q' \in f^{-1}(q)$,

$$\nu_q(\{q'\}) = \lim_{dq' \rightarrow \{q'\}} \frac{\lambda(dq')}{\mu(f(dq'))} = \left| \det(g_{\mathcal{Q}^{(n)}}(df(e_i), df(e_j)))_{i,j \leq \ell} \right|^{-1/2} \quad (74)$$

³Alternatively, ν_q can be expressed as a differential form $\hat{\nu}_q$ of maximal degree on S , $\hat{\nu}_q(q')(v_1, \dots, v_k) = \hat{\lambda}(q')(v_1, \dots, v_k, e_1, \dots, e_\ell)$ for any $q' \in S$ and $v_1, \dots, v_k \in T_{q'}S$, where $\hat{\lambda}$ is the differential form corresponding to the measure λ (i.e., the Riemannian volume form on $\partial\mathcal{Q}^{(n')}$), and the e_i are any vectors such that $df(e_1), \dots, df(e_\ell)$ is an orthonormal basis of $T_q\mathcal{Q}$.

for any orthonormal basis $\{e_i\}$ of the tangent space $T_{q'}\partial\mathcal{Q}$.

We now set up the Hamiltonian and IBC. We may include a potential, either as a function $V : \mathcal{Q} \rightarrow \mathbb{R}$ or more generally as a cross-section of $E \otimes E^*$ that is pointwise self-adjoint; here, E_q^* denotes the dual space of E_q , so an element $V(q)$ of $E_q \otimes E_q^*$ corresponds to an endomorphism $E_q \rightarrow E_q$ that we also denote by $V(q)$, and V being pointwise self-adjoint means that $V(q)$ is self-adjoint on E_q relative to $(\ , \)_q$.

The IBC demands that for every boundary point q ,

$$\left(\alpha(q) + \beta(q)\partial_n\right)\psi(q) = \frac{2}{\hbar^2}\psi(f(q)), \quad (75)$$

where $\alpha(q)$ and $\beta(q)$ are given complex-linear mappings $E_q \rightarrow E_{f(q)}$ and ∂_n means the normal derivative, i.e., the directional covariant derivative in the inward normal direction to the boundary at q (normal in terms of the Riemann metric g_{ij}).

The Hamiltonian is, for any interior point q :

$$H\psi(q) = -\frac{\hbar^2}{2}\Delta\psi(q) + V(q)\psi(q) + \int_{f^{-1}(q)} \nu_q(dq') \left(\gamma(q') + \delta(q')\partial_n\right)\psi(q'). \quad (76)$$

Here, Δ is the Laplace operator associated with the Riemannian metric of \mathcal{Q} and the connection of E (see, e.g., [4] for a detailed definition), and the coefficients $\gamma(q')$ and $\delta(q')$ are given complex-linear mappings $E_{q'} \rightarrow E_{f(q')}$. (The coefficient $\delta(q')$ should not be confused with a Dirac delta function.) The functions $\alpha, \beta, \gamma, \delta$ are required to satisfy at every $q \in \partial\mathcal{Q}$ the conditions

$$\alpha(q)^\dagger \gamma(q) : E_q \rightarrow E_q \text{ is self-adjoint relative to } (\ , \)_q \quad (77)$$

$$\beta(q)^\dagger \delta(q) : E_q \rightarrow E_q \text{ is self-adjoint relative to } (\ , \)_q \quad (78)$$

$$\alpha(q)^\dagger \delta(q) - \gamma(q)^\dagger \beta(q) = -I_{E_q}, \quad (79)$$

where I_{E_q} means the identity operator on E_q and $\alpha(q)^\dagger : E_{f(q)} \rightarrow E_q$ means the adjoint of $\alpha(q)$ relative to $(\ , \)_q$ and $(\ , \)_{f(q)}$, i.e.,

$$(\chi, \alpha(q)^\dagger \phi)_q = (\alpha(q)\chi, \phi)_{f(q)} \quad (80)$$

for any $\chi \in E_q$ and $\phi \in E_{f(q)}$; likewise for $\beta(q)^\dagger$.

We think of the masses as incorporated into the metric g_{ij} , as in, e.g.,

$$ds^2 = m_1 dx_1^2 + m_1 dy_1^2 + m_1 dz_1^2 + m_2 dx_2^2 + m_2 dy_2^2 + m_2 dz_2^2 \quad (81)$$

for two particles of different mass in Euclidean space (see [4] for further discussion). Then the mass need not be put into the prefactor of the Laplacian (in the Hamiltonian H as in (76) above) or the gradient (in the current j as in (84) below).⁴

⁴This convention has the possibly undesirable consequence that, when different sectors correspond to different particle number, the Riemannian volume μ is weighted in different sectors with different powers of the mass (such as m^{3n}); however, this can easily be compensated by reweighting $\psi^{(n)}$ by a factor of $m^{-3n/2}$, which in turn requires, if $f(q)$ contains one particle less than q , a further factor of $m^{-3/2}$ in $\alpha, \beta, \gamma, \delta$.

This completes the definition of the Hamiltonian. In contrast to Model 1 and Model 2 with IBCs, ψ does not diverge at the boundary in this case.

4.3 Conservation of Probability

Here is a formal (non-rigorous) derivation of the conservation of $|\psi|^2$, i.e., a check of self-adjointness of H on the non-rigorous level. By $|\psi|^2$, we mean $|\psi(q)|^2 = (\psi(q), \psi(q))_q$, which is the density relative to μ of the probability distribution in \mathcal{Q} associated with $\psi \in \mathcal{H}$ with $\|\psi\| = 1$. It evolves in general according to the balance equation

$$\frac{\partial |\psi(q)|^2}{\partial t} = \frac{2}{\hbar} \operatorname{Im}(\psi(q), H\psi(q))_q. \quad (82)$$

It is known (e.g., [4]) that for $H = -\frac{\hbar^2}{2}\Delta$ in a Hermitian vector bundle over a Riemannian manifold,

$$\frac{2}{\hbar} \operatorname{Im}(\psi(q), H\psi(q))_q = -\operatorname{div} j(q) \quad (83)$$

with the probability current vector field

$$j(q) = \hbar \operatorname{Im}(\psi(q), \nabla \psi(q))_q \quad (84)$$

on \mathcal{Q} . Here, $\operatorname{div} j$ denotes the divergence of the vector field j ; in coordinates, $\operatorname{div} j = \sum_a D_a j^a$, where D_a is the covariant derivative operator arising from the Riemann metric on \mathcal{Q} . The gradient $\nabla \psi$ is the E -valued vector field obtained from the E -valued 1-form that is the covariant derivative of ψ by “raising the index” using the Riemann metric.

Now for the Hamiltonian (76), the balance equation (82) becomes

$$\frac{\partial |\psi(q)|^2}{\partial t} = -\operatorname{div} j(q) + \int_{f^{-1}(q)} \nu_q(dq') \frac{2}{\hbar} \operatorname{Im}(\psi(q), [\gamma(q') + \delta(q')\partial_n]\psi(q'))_q. \quad (85)$$

For each q' , the integrand can be written, by virtue of the IBC (75), as

$$\begin{aligned} & \frac{2}{\hbar} \operatorname{Im}\left(\frac{\hbar^2}{2}[\alpha(q') + \beta(q')\partial_n]\psi(q'), [\gamma(q') + \delta(q')\partial_n]\psi(q')\right)_q \\ &= \hbar \operatorname{Im}\left(\psi(q'), \alpha(q')^\dagger \gamma(q')\psi(q')\right)_{q'} \\ &+ \hbar \operatorname{Im}\left(\psi(q'), \alpha(q')^\dagger \delta(q')\partial_n \psi(q')\right)_{q'} \\ &- \hbar \operatorname{Im}\left(\psi(q'), \gamma(q')^\dagger \beta(q')\partial_n \psi(q')\right)_{q'} \\ &+ \hbar \operatorname{Im}\left(\partial_n \psi(q'), \beta(q')^\dagger \delta(q')\partial_n \psi(q')\right)_{q'}, \end{aligned} \quad (86)$$

where the first and the last term vanish by virtue of (77) and (78). What remains is

$$\hbar \operatorname{Im}\left(\psi(q'), [\alpha(q')^\dagger \delta(q') - \gamma(q')^\dagger \beta(q')] \partial_n \psi(q')\right)_{q'}, \quad (88)$$

which agrees, by virtue of (79), with

$$-\hbar \operatorname{Im} \left(\psi(q'), \partial_n \psi(q') \right)_{q'} = -j_n(q'), \quad (89)$$

where $j_n(q')$ means the component of $j(q')$ normal to the boundary, or

$$j_n = j^i n^j g_{ij} \quad (90)$$

with n the inward-pointing unit normal vector to the boundary. Thus, in total,

$$\frac{\partial |\psi(q)|^2}{\partial t} = -\operatorname{div} j(q) - \int_{f^{-1}(q)} \nu_q(dq') j_n(q'). \quad (91)$$

Now, if $j_n(q') < 0$ then $-j_n(q') \lambda(dq') dt$ is the amount of $|\psi|^2$ weight lost in the sector containing q' due to current into the boundary region dq' around q' within duration dt . Likewise, if $j_n(q') > 0$ then $j_n(q') \lambda(dq') dt$ is the amount of $|\psi|^2$ weight *gained* in the sector containing q' due to current coming from dq' within duration dt . That is, $j_n(q') \lambda(dq') dt$ is the net gain, positive or negative. Now the second term on the right-hand side of (91) represents a gain in the amount of $|\psi|^2$ weight (while the $\operatorname{div} j$ term represents transport of $|\psi|^2$ weight within one sector); in fact, the gain in the region dq around q within duration dt is

$$-\mu(dq) dt \int_{f^{-1}(q)} \nu_q(dq') j_n(q') = -dt \int_{f^{-1}(dq)} \lambda(dq') j_n(q'). \quad (92)$$

Thus, the net gain in dq exactly compensates the net loss in $f^{-1}(dq)$, and $\|\psi\|^2 = \int_{\mathcal{Q}} |\psi(q)|^2 \mu(dq)$ is conserved.

Equation (91) can be regarded as a transport equation for the $|\psi|^2$ weight, with two types of transport: continuous motion within a sector of \mathcal{Q} , and transport between sectors of \mathcal{Q} (either from q' to $f(q')$ or from $f(q')$ to q'). Equation (91) actually is a probability transport equation for the $|\psi|^2$ -distributed stochastic process in \mathcal{Q} described in [5].

It also becomes clear from the above derivation of (91) that the conditions (77), (78), and (79) cannot be weakened within our scheme without losing (91) and thus the self-adjointness of H . (Except that (77)–(79) may fail on a λ -null set of boundary configurations, or $\alpha, \beta, \gamma, \delta$ may be undefined on such a set.) After all, if $\psi(q')$ and $\partial_n \psi(q')$ can be chosen independently, then the only way in which (86) can always be equal to (89) is if (77), (78), and (79) are true. Now $\psi(q')$ and $\partial_n \psi(q')$ can be chosen independently by appropriate choice of initial data for ψ —despite the IBC (75), which can be satisfied by appropriate choice of $\psi(f(q'))$. To be sure, (91) can be true for all ψ satisfying the IBC also if the integrals in (85) and (91) agree while the integrands are not equal. For example, this happens when $\gamma = 0 = \delta$ (so (79) is violated), $f^{-1}(q)$ contains two boundary points, say q' and q'' , and the loss at q' always compensates the gain at q'' and vice versa (e.g., if $j_n(q') = -j_n(q'')$ and $\nu_q(\{q'\}) = \nu_q(\{q''\})$). However, such possibilities lie outside our scheme, according to which the weight lost at q' is added to $f(q')$, and will not be considered here.

4.4 Application: Cut-Off Radius

IBCs on a codimension-1 boundary can be used for implementing an unusual kind of UV cut-off, in which the x -particle is smeared out, but not over a ball but over a sphere of small radius $\delta > 0$. While an x -particle smeared out over a ball can emit and absorb y -particles anywhere within that ball, an x -particle smeared out over a sphere can only emit and absorb y -particles at a distance from its center that is exactly δ . That is, a y -particle gets absorbed as soon as it reaches distance δ from the center of an x -particle, and gets created on the sphere of radius δ . We exclude the possibility that any y -particle is ever closer than δ to an x -particle. This kind of UV cut-off was first described, as far as we know, in [18]; we will call it a “ δ -cut-off” in the following.

When we apply this cut-off to Model 1, the configuration space is

$$\mathcal{Q} = \left\{ (x^m, y^n) \in \mathcal{Q}_x \times \mathcal{Q}_y : |\mathbf{x}_i - \mathbf{y}_j| \geq \delta \forall i, j \right\} \quad (93)$$

with \mathcal{Q}_x and \mathcal{Q}_y as in (6), and its boundary

$$\partial \mathcal{Q} = \left\{ (x^m, y^n) \in \mathcal{Q} : |\mathbf{x}_i - \mathbf{y}_j| = \delta \text{ for some } i, j \right\} \quad (94)$$

has codimension 1 almost everywhere. For Model 2, the configuration space would be

$$\mathcal{Q} = \left\{ y^n \in \mathcal{Q}_y : |\mathbf{y}_j| \geq \delta \forall j \right\} \quad (95)$$

with boundary

$$\partial \mathcal{Q} = \left\{ y^n \in \mathcal{Q}_y : |\mathbf{y}_j| = \delta \text{ for some } j \right\} \quad (96)$$

(also of codimension 1), and the Hilbert space is $\mathcal{H} = L^2(\mathcal{Q})$. Let B_δ denote the δ -ball around the origin, $B_\delta = \{\mathbf{y} \in \mathbb{R}^3 : |\mathbf{y}| < \delta\}$.

The IBC (for simplicity for Model 2 with δ -cut-off) of Dirichlet type demands the following: For every $\boldsymbol{\omega} \in \mathbb{S}^2$, $n \in \{0, 1, 2, \dots\}$, $y^n \in (\mathbb{R}^3 \setminus B_\delta)^n$,

$$\psi^{(n+1)}(y^n, \delta \boldsymbol{\omega}) = -\frac{g m_y}{2\pi \hbar^2 \delta \sqrt{n+1}} \psi^{(n)}(y^n). \quad (97)$$

The associated Hamiltonian is defined by

$$\begin{aligned} (H\psi)^{(n)}(y^n) &= -\frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi^{(n)}(y^n) + nE_0 \psi^{(n)}(y^n) \\ &\quad + \frac{g\sqrt{n+1}}{4\pi} \int_{\mathbb{S}^2} d^2\boldsymbol{\omega} \left. \frac{\partial}{\partial r} \right|_{r=\delta} \left(r \psi^{(n+1)}(y^n, r\boldsymbol{\omega}) \right) \end{aligned} \quad (98)$$

at any $y^n \in \mathcal{Q} \setminus \partial \mathcal{Q}$.

In the language of Sections 4.1–4.3, $g_{ij} = m_y \delta_{ij}$, $f(y^n) = y^n \setminus B_\delta$, the Hermitian vector bundle E is the trivial rank-1 bundle $E = \mathcal{Q} \times \mathbb{C}$, μ is the volume as in (7),

$$\partial \mathcal{Q}^{(n)} = \bigcup_{j=1}^n (\mathbb{R}^3 \setminus B_\delta)^{j-1} \times \mathbb{S}_\delta^2 \times (\mathbb{R}^3 \setminus B_\delta)^{n-j}, \quad (99)$$

λ is locally $\text{vol}_{3(j-1)} \times \text{area} \times \text{vol}_{3(n-j)}$,

$$f^{-1}(y^n) = \bigcup_{j=1}^n \{(\mathbf{y}_1, \dots, \mathbf{y}_j - 1, \delta \boldsymbol{\omega}, \mathbf{y}_j, \dots, \mathbf{y}_n) : \boldsymbol{\omega} \in \mathbb{S}^2\}, \quad (100)$$

$\nu_{y^n}(d^2 \boldsymbol{\omega}) = \delta^2 d^2 \boldsymbol{\omega}$ on any of the n spheres in (100), $\alpha(y^n) = -4\pi\delta\sqrt{n+1}/gm_y$, $\beta(y^n) = 0$, $\gamma(y^n) = 0$, and $\delta(y^n) = gm_y/4\pi\delta\sqrt{n+1}$.

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